

# MULTISCALE ANALYSIS OF A DAVYDOV MODEL WITH AN HARMONIC LONG RANGE INTERACTION OF KAC-BAKER TYPE

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## Abstract

The classical equation of motion of a Davydov model in a coherent state approximation is analyzed using the multiple scales method. An exponentially decaying long range interaction (Kac-Baker model) was included. In the first order, the dominant amplitude has to be a solution of the nonlinear Schrödinger equation (NLS). In the next order the second amplitude satisfies an inhomogeneous linearized NLS equation, the inhomogeneous term depending only on the dominant amplitude. In order to eliminate possible secular behaviour the dominant amplitude has to satisfy also the next equation in the NLS hierarchy (a complex modified KdV equation). When the second order derivative of the dispersion relation vanishes the scaling of the slow space variable has to be changed, and a generalized NLS equation with a third order derivative is found for the dominant amplitude. As the coefficient of the third derivative is small a perturbational approach is used to discuss the equation. A complete solution is given when the dominant amplitude is the one-soliton solution of the NLS equation.

## 1. Introduction

Many quasi-one-dimensional molecular systems are very complicated structures built from complexes of atoms - we call them "molecules" - connected by hydrogen bonds. As an example we mention the complicate structure of  $\alpha$ -helix in protein. A very simple model consists in replacing the three coupled chains of the complex  $\alpha$ -helix structure by only one chain of the form  $\dots H - N - C = O - H - N - C = O \dots$ . Also only one of the intramolecular excitations - that corresponding to the amide I oscillation - is taken into account (further on they will be called vibrons). An acoustic phonon field describing the oscillations of the molecules along the chain is also introduced. As the amide I oscillation energy depends on the stretching of the adjacent hydrogen bond an anharmonic interaction between vibrons and phonons appears.

It is now easy to write an Hamiltonian of Fröhlich type for this very simplified model. For a system with a conserved number of vibrons the model was proposed by Davydov [1]-[4] more than 25 years ago. Eliminating this constraint of fixed number of vibrons the model was extended by Takeno [5],[6],[3] at the beginning of the eighties.

The Hamiltonian of Davydov's model is given by

$$\begin{aligned}\hat{H} &= \sum_n E B_n^+ B_n - \sum_{n \neq m} J_{mn} (B_n^+ B_m + B_m^+ B_n) \\ &+ \sum_n \left( \frac{1}{2m} \hat{p}_n^2 + \frac{1}{2} w (\hat{u}_{n+1} - \hat{u}_n)^2 \right) + \chi \sum_n (\hat{u}_{n+1} - \hat{u}_n) B_n^+ B_n.\end{aligned}\quad (1)$$

Here  $B_n, B_n^+$  are the annihilation/creation operators for vibronic excitation of energy  $E$  in the cell  $n$ ,  $J_{mn}$  term takes into account the long range interaction between vibrons,  $\hat{u}_n, \hat{p}_n$  are the displacement operator and the corresponding conjugate momentum of the  $n$ -th molecule,  $m$  is an effective mass of the molecule,  $w$  the elastic constant and  $\chi$  a coupling constant describing the nonlinear interaction between vibrons and phonons. As an example of the long range interaction between vibrons we shall consider an exponentially decreasing model (Kac-Baker model) [7]

$$J_{mn} = J \frac{1-r}{2r} e^{-\gamma|m-n|}, \quad r = e^{-\gamma}. \quad (2)$$

Since the pioneering paper of Sarker and Krumhansl [8] this model was intensively used by a series of authors to investigate the thermodynamic properties and the soliton characteristics in several nonlinear 1-D systems [9] - [14].

It is a general belief that a coherent state approximation is very suitable for describing extended localized states in such systems. Such an hypothesis was done by Davydov. His ansatz for the state vector is

$$|\Psi(t)\rangle = \sum_n a_n(t) B_n^+ \exp \left( -\frac{i}{\hbar} \sum_j \beta_j(t) \hat{p}_j - \pi_j(t) \hat{u}_j \right) |0\rangle, \quad (3)$$

$|0\rangle$  being the vacuum state both for vibrons and phonons. Here  $a_n(t), \beta_n(t), \pi_n(t)$  are now  $c$ -numbers, time depending, which will be determined from a variational principle. Using the average value of  $\hat{H}$  as Hamiltonian in the classical equations of motion one gets

$$\begin{aligned}i\hbar \dot{a}_n &= E a_n - \sum_{p=1}^{\infty} J_p (a_{n+p} + a_{n-p}) + \chi (\beta_{n+1} - \beta_n) a_n \\ M \ddot{\beta} &= w (\beta_{n+1} - 2\beta_n + \beta_{n-1}) + \chi (|a_n|^2 - |a_{n-1}|^2).\end{aligned}\quad (4)$$

In an adiabatic approximation ( $\dot{\beta}_n \rightarrow 0$ ) from the second eq. (4) we get

$$\beta_{n+1} - \beta_n = -\frac{\chi}{w} |a_n|^2,$$

which introduced into the first gives

$$i\hbar\dot{a}_n = Ea_n - \sum J_p(a_{n+p} + a_{n-p}) - \frac{\chi^2}{w}|a_n|^2a_n. \quad (5)$$

a typical self-trapping equation.

## 2. Multiple scale approach

The linearized problem admits plane wave solutions with the dispersion relation

$$\hbar\omega(k) = E - J\frac{1-r}{2r}\sum_{p=1}^{\infty}e^{-\gamma p}\cos klp = E - J\frac{1-r}{2r}\left(\frac{\sinh\gamma}{\cosh\gamma - \cos kl} - 1\right). \quad (6)$$

A plane wave solution with constant amplitude exists even for the nonlinear equation (5), but with an amplitude depending dispersion relation (Stokes waves)

$$\hbar\omega(k) = E - J\frac{1-r}{2r}\sum_p e^{-\gamma p}\cos klp - \frac{\chi^2}{w}|a|^2. \quad (7)$$

It is well known that these solutions are unstable at small modulation of the amplitude (Benjamin Feir instability) [15]. To see this in our case we write

$$a_n = a(1 - \mathcal{A}_n(t))e^{i(kln - \omega t)}$$

where  $\mathcal{A}_n(t)$  are satisfying the following system of linear equations

$$i\hbar\dot{\mathcal{A}}_n = 2\sum J_p\mathcal{A}_n\cos klp - \sum J_p(\mathcal{A}_{n+p}e^{iklp} + \mathcal{A}_{n-p}e^{-iklp}) - \frac{\chi^2}{w}|a|^2(\mathcal{A}_n + \mathcal{A}_n^*).$$

Looking for plane wave solutions

$$\mathcal{A}_n = ce^{i(\nu ln - \Omega t)} + de^{-i(\nu ln - \Omega t)}$$

the instability,  $\Omega^2 < 0$ , appears when

$$\left(\sum_p J_p\cos klp(1 - \cos \nu lp)\right)\left(\sum_p J_p\cos klp(1 - \cos \nu lp) - \frac{\chi^2}{w}|a|^2\right) \leq 0$$

which is always satisfied at small wave numbers  $\nu$ .

In order to describe this process of amplitude modulation, the multiple scales approach (reductive perturbative method) [16]-[20] is used. The solution is written as an asymptotic expansion in a small parameter  $\epsilon$ .

$$a_n = e^{i(kln - \omega t)}\sum_j \epsilon^j A_j(\xi, t_2, t_3, \dots) \quad (8)$$

where the amplitudes  $A_j$  depend on some slow variables  $\xi, t_2, t_3, \dots$ . In order to see how these can be defined let us expand the dispersion relation around a point  $k_0$  ( $k = k_0 + \Delta k$ )

$$\omega(k) = \omega_0 + \omega_1 \Delta k + \omega_2 \Delta k^2 + \dots, \quad \omega_n = \frac{1}{n!} \frac{d^n \omega(k)}{dk^n} \Big|_{k=k_0}$$

and considers  $\Delta k = \mu \epsilon^\alpha$ . Then the phase of the plane wave can be written

$$kln - \omega t = (k_0 ln - \omega_0 t) + \mu \epsilon^\alpha (ln - \omega_1 t) - \mu^2 \omega_2 \epsilon^{2\alpha} t - \mu^3 \omega_3 \epsilon^{3\alpha} t + \dots \quad (9)$$

Two distinct situations can appear. In the first case  $\omega_2 \neq 0$  (we shall call it "a normal situation") and the second when  $\omega_2 = 0$ . This last situation is referred as the "zero dispersion point" case (ZDP). In the normal situation, with  $\alpha = 1$ , and the following definition of the slow variables

$$\xi = \epsilon(ln - v_g t), \quad \tau_2 = \epsilon^2 t, \quad \tau_3 = \epsilon^3 t, \dots \quad (10)$$

it is easily seen that a competition between nonlinearity,  $\frac{\partial A_1}{\partial \tau_2}$  and  $\frac{\partial^2 A_1}{\partial \tau_2^2}$  will occur in order  $\epsilon^3$ . Introducing these in (5) we ask that the equation has to be satisfied in each order of  $\epsilon$ . In the first order in  $\epsilon$  the equation is linear and we obtain the dispersion relation (6). In the next order  $\epsilon^2$  the equation is satisfied if the velocity  $v_g$  is given by  $v_g = \omega_1$ . In the order  $\epsilon^3$  we found that the leading amplitude  $A_1$  has to satisfy the well known nonlinear Schrödinger equation (NLS)

$$\frac{\partial A_1}{\partial \tau_2} + \omega_2 \left( \frac{\partial^2 A_1}{\partial \xi^2} + 2c|A_1|^2 A_1 \right) = 0, \quad c = \frac{q}{2\omega_2}, \quad q = \frac{\chi^2}{\hbar w}. \quad (11)$$

Recently [21] the analysis for Takeno's model was extended to the next order  $\epsilon^4$ . Similarly, in the present case, a nonhomogeneous linear equation satisfied by the next amplitude  $A_2$  is obtained, namely

$$i \frac{\partial A_2}{\partial \tau_2} + \omega_2 \frac{\partial^2 A_2}{\partial \xi^2} + q(A_1^2 A_2^* + 2|A_1|^2 A_2) = -i \frac{\partial A_1}{\partial \tau_3} + i\omega_3 \frac{\partial^3 A_1}{\partial \xi^3}. \quad (12)$$

In the left hand side (lhs) we recognize the linearized NLS equation (l-NLS eq.), while the nonhomogeneity in the right hand side (rhs) contains only the dominant amplitude  $A_1$ , solution of the NLS eq. In solving the equation (12) we are confronted with two distinct problems. Firstly we have to take care to eliminate any secular behaviours raised by the presence of the nonhomogeneity. They can appear from terms in the rhs which are members of the null space of the l-NLS eq. As is well known the symmetries of the NLS eq. are solutions of the l-NLS eq., so the dangerous terms in the rhs of (12) are to be found between them. Such a symmetry is easily identified in (12) namely

$$\sigma_3 = - \left( \frac{\partial^3 A_1}{\partial \xi^3} + 6c|A_1|^2 \frac{\partial A_1}{\partial \xi} \right) \quad (13)$$

and the possible secular behaviour is eliminated if the  $\tau_3$  dependence of  $A_1$  is given by

$$-\frac{\partial A_1}{\partial \tau_3} + \omega_3 \left( \frac{\partial^3 A_1}{\partial \xi^3} + 6c|A_1|^2 \frac{\partial A_1}{\partial \xi} \right) = 0. \quad (14)$$

This is a complex modified KdV equation and is the second equation in the hierarchy associated to NLS eq. As all the equations in the hierarchy have the same spectral problem the  $\tau_3$  time dependence of  $A_1$  can appear only in the initial positions and phases characterizing the solution  $A_1$  of the NLS eq. After this "renormalization" of the dominant amplitude  $A_1$  we remain with a nonhomogeneous linear equation, free of secularities, for the second amplitude  $A_2$

$$i \frac{\partial A_2}{\partial \tau_2} + \omega_2 \frac{\partial^2 A_2}{\partial \xi^2} + q(A_1^2 A_2^* + 2|A_1|^2 A_2) = -6i\omega_3 c |A_1|^2 \frac{\partial A_1}{\partial \xi}. \quad (15)$$

A simple method to solve it when  $A_1$  is the one-soliton solution of NLS eq. will be given in the next section. More comments will be presented there.

In the last years several papers have discussed the significance of the higher order approximations to a nonlinear dynamical problem, which in the lowest relevant order is described by a completely integrable equation [22]-[24], and the role played by the next equations from the corresponding hierarchies in order to eliminate possible secular behaviours. Our results are in completely agreement with these discussions.

### 3. ZDP case

Let us discuss now the case of zero dispersion point. For models in which the carrier wave is of the form of a lattice plane wave such a point  $k_0$  exist always in the first Brillouin zone. It corresponds to the maximum group velocity of the localized excitation. For the dispersion relation (6) it is given by

$$\cos k_0 l = \frac{1}{2} \left( \sqrt{\cosh^2 \gamma + 8} - \cosh \gamma \right). \quad (16)$$

The analysis presented in the previous paragraph has to be slightly modified. In the phase (9) the  $\omega_2$  term is missing. Then the next term has to be used to define the time variable  $\tau_2$  and consequently we have to consider  $\alpha = \frac{2}{3}$ . The slow variables are now given by

$$\xi = \epsilon^{\frac{2}{3}}(ln - \omega_1 t), \quad \tau_2 = \epsilon^2 t. \quad (17)$$

In order  $\epsilon^3$  we shall have a competition between the nonlinearity, the time derivative  $\frac{\partial A_1}{\partial \tau_2}$  and the third order spatial derivative  $\frac{\partial^3 A_1}{\partial \xi^3}$ . Also the second derivative  $\frac{\partial^2 A_1}{\partial \xi^2}$  can contribute in the same order  $\epsilon^3$  because it is multiplied by  $\omega_2(k)$ , which

expanded around  $k_0$  brings an extra  $\epsilon^{\frac{2}{3}}$  dependence ( $\omega_2(k) = 3\omega_3\mu\epsilon^{\frac{2}{3}} + \dots$ ). Collecting all these contributions of  $\epsilon^3$  order we arrive at the following equation satisfied by the dominant amplitude  $A_1$

$$i\frac{\partial A_1}{\partial \tau_2} + 3\mu\omega_3\frac{\partial^2 A_1}{\partial \xi^2} + q|A_1|^2 A_1 = i\omega_3\frac{\partial^3 A_1}{\partial \xi^3}. \quad (18)$$

Introducing dimensionless quantities

$$X = \frac{1}{\sqrt{6\mu}}k_0\xi, \quad T = \omega_3k_0^3\tau_2, \quad \Psi = \sqrt{\frac{\chi^2}{\hbar\omega_3k_0^3w}}A_1 \quad (19)$$

the equation (18) becomes

$$I\frac{\partial \Psi}{\partial T} + \frac{1}{2}\frac{\partial^2 \Psi}{\partial X^2} + |\Psi|^2\Psi = i\beta\frac{\partial^3 \Psi}{\partial X^3} \quad (20)$$

where  $\beta = (6\mu)^{-\frac{3}{2}}$ . This is a NLS eq. perturbed with a third order derivative term. As  $\beta$  is small the eq. (20) will be solved by a perturbation approach. We consider

$$\Psi \rightarrow \Psi + \beta\delta\Psi \quad (21)$$

where now  $\Psi$  is a solution of the unperturbed NLS eq. Also we introduce a slow time variable  $\tau = \beta T$ . In first order in  $\beta$  we get

$$i\frac{\partial \delta\Psi}{\partial T} + \frac{1}{2}\frac{\partial^2 \delta\Psi}{\partial X^2} + (2|\Psi|^2\delta\Psi + \Psi^2\delta\Psi^*) = -i\frac{\partial \Psi}{\partial \tau} + i\frac{\partial^3 \Psi}{\partial X^3}. \quad (22)$$

This equation is exactly of the same form as (12). The possible secular behaviour is eliminated requiring that the  $\tau$  dependence of  $\Psi$  is given by the complex mKdV equation

$$-\frac{\partial \Psi}{\partial \tau} + \frac{\partial^3 \Psi}{\partial X^3} + 6|\Psi|^2\frac{\partial \Psi}{\partial X} = 0. \quad (23)$$

We remain with a linear nonhomogeneous equation for  $\delta\Psi$  namely

$$i\frac{\partial \delta\Psi}{\partial T} + \frac{1}{2}\frac{\partial^2 \delta\Psi}{\partial X^2} + (2|\Psi|^2\delta\Psi + \Psi^2\delta\Psi^*) = -6i|\Psi|^2\frac{\partial \Psi}{\partial X} \quad (24)$$

which is free of secularities.

Further we shall give a complete solution for the case when  $\Psi$  is the one-soliton solution of the NLS eq. If  $z = u + iv$  is the eigenvalue of the spectral problem the one soliton solution is given by

$$\Psi = 2v\frac{e^{-i\Phi}}{\cosh \Theta}, \quad \Phi = 2uX + 2(u^2 - v^2)T + \Phi_0, \quad \Theta = 2v(X - X_0 + 2uT). \quad (25)$$

As mentioned before, the  $\tau$ -dependence can appear only in the initial phase  $\Phi_0$  and the initial position  $X_0$ . Introducing (25) in (23) it is easily find that

$$\frac{d\Phi_0}{d\tau} = 8u(u^2 - 3v^2), \quad \frac{dX_0}{d\tau} = 4(3u^2 - v^2) \quad (26)$$

which lead to a linear dependence of  $\Phi_0$  and  $X_0$  on the slow time variable  $\tau$ .

As is well known the NLS eq. is invariant under Galilei transformation. The same is true also for the l-NLS eq., so without any lost of generality we can solve (24) in the reference frame where the soliton is at rest ( $u = 0$ ) and then through the Galilei transformation

$$X = X' + 2uT', \quad T = T', \quad \delta\Psi = \delta\Psi' e^{(2iuX' + 2iu^2T')} \quad (27)$$

we can find the solution in the laboratory system. The one-soliton solution in its own reference frame is given by

$$\Psi = 2v \frac{e^{2iv^2T}}{\cosh 2vX}. \quad (28)$$

We are looking for solutions of the form

$$\delta\Psi = ie^{2iv^2T}Y(X) \quad (29)$$

with  $Y(X)$  a real function. With  $2vX \rightarrow X$  and introducing the new variable  $\rho = \tanh X$  the equation satisfied by  $Y$  becomes

$$\frac{d}{d\rho} \left( (1 - \rho^2) \frac{dY}{d\rho} \right) + \left( 2 - \frac{1}{1 - \rho^2} \right) Y = 48v^2 \rho \sqrt{1 - \rho^2}. \quad (30)$$

In the lhs we recognize the equation for the associated Legendre polynomials. The two linear independent solutions are  $P_1^1$  and  $Q_1^1$

$$P_1^1 = -\sqrt{1 - \rho^2}, \quad Q_1^1 = -\sqrt{1 - \rho^2} \left( \frac{1}{2} \ln \frac{1 + \rho}{1 - \rho} + \frac{\rho}{1 - \rho^2} \right). \quad (31)$$

We write the solution of the nonhomogeneous equation (30) as a linear superposition

$$Y(\rho) = \alpha(\rho)P_1^1(\rho) + \beta(\rho)Q_1^1(\rho), \quad (32)$$

where  $\alpha(\rho), \beta(\rho)$  are coefficients to be determined. A general way to find them is to consider

$$\frac{d\alpha}{d\rho} = fQ_1^1, \quad \frac{d\beta}{d\rho} = fP_1^1. \quad (33)$$

Then using the Wronskian expression it is easily found that

$$f(\rho) = -24v^2 \rho \sqrt{1 - \rho^2}. \quad (34)$$

Then the equations for  $\alpha$  and  $\beta$  are easily integrated giving

$$\alpha(\rho) = -3v^2(1 - \rho^2)^2 \ln \frac{1 + \rho}{1 - \rho} + 6v^2\rho(1 + \rho^2), \quad \beta(\rho) = 6v^2(1 - \rho^2). \quad (35)$$

In integrating the equation for  $\beta$  an integration constant was determined from the condition  $\beta(\pm 1) = 0$ . This ensure us to have  $Y(\rho)$  finite everywhere for  $\rho \in [-1, +1]$ . Now introducing (35) in (32) a very simple form for  $Y(\rho)$  is found, namely

$$Y(\rho) = -12v^2\rho\sqrt{1 - \rho^2}. \quad (36)$$

As  $Y(\rho)$  is zero both in the origin and at  $\rho = \pm 1$  ( $X \rightarrow \pm\infty$ ) it has a maximum at  $\rho = \pm \frac{1}{\sqrt{2}}$ , which transformed in the  $X$  variable gives  $X = \frac{1}{2v} \ln(1 + \sqrt{2})$ . This maximum is similar with that found in numerical simulations and other theoretical treatments of the similar ZDP problem of pulse propagation in nonlinear optical fibers [25]-[29].

#### 4. Conclusions

Solitonic type excitations in a Davydov model are investigated. The multiple scales method is used to study the space-time modulation of the amplitude. As expected the dominant amplitude  $A_1$  is satisfying a NLS eq. In the next order the second amplitude  $A_2$  is given by the solution of a nonhomogeneous linearized NLS equation. Possible secular behaviours are generated if symmetries of NLS eq. are identified in the rhs of this equation. They are eliminated if the NLS solution satisfies also the next eq. in the NLS hierarchy (a complex mKdV equation). The ZDP case is also investigated using the same method of multiple scales, but with another definition of the slow spatial variable. The dominant amplitude satisfies a modified NLS equation containing a third order derivative term. As its coefficient is a small quantity a perturbational approach is used. The case of the one-soliton solution of the NLS eq. is fully solved. Possible secular behavior is eliminated if the one-soliton solution satisfies also the next equation in the NLS hierarchy. A linear  $\tau_3$  dependence of the initial phase and position of the soliton is determined. The remaining equation, by a suitable transformation, is reduced to the equation for associated Legendre polynomials. The complete solution is found if the NLS soliton is at rest. By a Galilei transformation the solution for moving soliton is obtained. More complicated situations are under investigation.

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